Journal of Computational Chemistry

Volume 8 Number 1 January/February 1987

Recursion Formulae for Calculation of Overlap Integrals
N. C. Datta and B. Sen 1

The Role of *d* Functions in *AB-INITIO* Calculations. II. The Deformation Densities of SO_2, NO_2, and Their Ions
D. W. J. Cruickshank and M. Eisenstein 6

Molecular Modeling of Polymers: I. Correct and Efficient Enumeration of Intrachain Conformational Energetics
B. J. Orchard, S. K. Tripathy, R. A. Pearlstein, and A. J. Hopfinger 28

Recent Advances in Multireference Second Order Perturbation CI: The CIPSI Method Revisited
R. Cimiraglia and M. Persico 39

On The Importance of Size-Consistency Corrections in Semiempirical MNDOC Calculations
D. Cremer and W. Thiel 48

Ab Initio Studies on Van Der Waals Molecules. A Comparative Study with Several Basis Sets of the *C2v* HeLi2 System
M. Matias, L. M. Tel, and J. J. Novoa 51

Hydration Structures and Energetics of Phospholipid
K. S. Kim and E. Clementi 57

Theoretical Study of Water-Pyridine Complexes Using Intermolecular Potentials
M. Genest 67

Polarization Counterpoise Corrections to Correlated Hydrogen Bond Interaction Energies
S. K. Loushin and C. E. Dykstra 81

Ab Initio Calculations on the Effect of Polarization Functions on Disiloxane
S. Grigoras and T. H. Lane 84

Volume 8 Number 2 March 1987

Optimized Method for the Evaluation of the Convolutionally Distorted Decay Curves
J. Szöke 95

Combination of MOMM and VEH Methods to Calculate Electronic Properties of Polymers
L. A. Burke, J. Kao, and A. C. Lilly, Jr. 107

Reliable Gaussian Basis Sets for Closed-Shell Atoms
E. Radzio and J. Andzelm 117

The Ellipsoid Algorithm as a Method for the Determination of Polypeptide Conformations from Experimental Distance Constraints and Energy Minimization
M. Billeter, T. F. Havel, and K. Wüthrich 132

Comparison of the Use of the MNDO and MINDO/3 Methods with *Ab Initio* Methods to Study Tautomerism in Histamine, 2- and 4-Methylhistamine
S. Topiol 142

Quantum Mechanical Modeling of a Transannular Interaction in a Bicyclic Amidinium Ion
W. D. Edwards and G. R. Weisman 149

Theoretical Study on the Mechanism of the Thermal Decarboxylation of Acrylic and Benzoic Acids. Models for Aqueous Solution
P. Ruelle 158

An Algorithm for Construction of the Molecular Distance Matrix
W. R.Müller, K. Szymanski, J. V. Knop, and N. Trinajstić 170

Molecular Mechanics and the Deformation of Macromolecules: The Use of a Very Short Cutoff Combined with a Quadratic Approximation
H. R. Karfunkel 174

Book Review 185

Announcements 186

Information for Contributors 187

Volume 8 Number 3 April/May 1987

Enumeration and Classification of Benzenoid Hydrocarbons
J. Brunvoll, S. J. Cyvin, and B. N. Cyvin 189

Electronic Structure of Clusters Modeling Silica
J. P. Lopez, C. Y. Yang, and C. R. Helms 198

Small Imines and Oximes as Model Compounds in the Optimization of a Consistent Force Field Potential Energy Function
C. J. M. Huige, A. M. F. Hezemans, and K. Rasmussen 204

Model Potentials for Molecular Calculations. I. The *sd*-MP Set for Transition Metal Atoms Sc through Hg
Y. Sakai, E. Miyoshi, M. Klobukowski, and S. Huzinaga 226

Model Potentials for Molecular Calculations. II. The *spd*-MP Set for Transition Metal Atoms Sc through Hg
Y. Sakai, E. Miyoshi, M. Klobukowski, and S. Huzinaga 256

The Through-Space Transmission of $^{77}Se—^{77}Se$ Coupling Constants
R. H. Contreras, H. O. Gavarini, and M. A. Natiello 265

Interaction Energy Studies of 8-Azapurine during Transcription
N. K. Sanyal, R. P. Ojha, and M. Roychoudhury 272

Volume 8 Number 4 June 1987

Introduction
P. G. Mezey 281

Converged Calculations of Rotational Energy Transfer in HF—HF Collisions
D. W. Schwenke and D. G. Truhlar 282

On Madelung's Constant
K. F. Taylor 291

Transition Structure in a Diabatic Surface Formalisom
F. Bernardi, J. J. W. McDouall, and M. A. Robb 296

Centrifugal Distortions in Molecules: An Ab Initio Approach with Application to Ozone
L. L. Lohr and A. J. Helman 307

Coupled Equations Approach to Multiphoton Molecular Processes
A. D. Bandrauk and N. Gélinas 313

Implementation and Applications of Gaussian 82 on a CDC Cyber 205
A. Rauk and R. Dutler 324

Simulation Studies of Branched Polymer Molecules
J. E. G. Lipson 333

Chemical Applications of Topology and Group Theory. 23. A Comparison of Graph-Theoretical and Extended Hückel Methods for Study of Bonding in Octahedral and Icosahedral Boranes
R. B. King 341

Generalized Potential Surfaces under Inclusion of Nuclear Motion
T. Krüger and K. Jug 350

Analysis of the π-Electronic Structure of Infinitely Large Networks. I. Some Remarks on the Characteristic Polynomial and Density of States of Large Polycyclic Aromatic Hydrocarbons
H. Hosoya, M. Aida, R. Kumagai, and K. Watanabe 358

Linear Notations and Molecular Graph Similarity
W. C. Herndon and S. H. Bertz 367

The Density Amplitude $\rho^{1/2}$ and the Potential which Generates It
N. H. March 375

Character Tables and Symmetry Eigenvectors for Two C_{3v} Rotor Molecular Systems
Y. G. Smeyers and A. Niño 380

Computational Studies of 1,2-Dithiete and Dithioglyoxal
J. D. Goddard 389

PERTURB: A Special-Purpose Algebraic Manipulation Program for Classical Perturbation Theory
L. E. Fried and G. S. Ezra 397

Time Step Error in Diffusion Monte Carlo Simulations: An Empirical Study
S. M. Rothstein, N. Patil, and J. Vrbik 412

Computational Aspects of Master Equation Transformation in Terms of Moments
G. Gidiotis and W. Forst 420

Discrete Models of Growth and Dynamical Percolation in Chemistry
S. J. Fraser 428

The Application of Strictly Localized Geminals to the Description of Chemical Bonds
R. A. Poirier and P. R. Surján 436

Application of the MuMATH Computer Algebra System to Sets of First Order Kinetic Equations of Significance in Chemistry
C. Trindle 442

Open-Shell Coupled-Cluster Method: Electron Affinities of Li and Na*
U. Kaldor 448

On the SCF Calculation of Excited States: Singlet States in the Two-Electron Problem
M. McCourt and J. W. Iver, Jr. 454

Numerical Calculation of Eigenvalues for the Schrödinger Equation. III
J. W. Neuberger and D. W. Noid 459

The Shape of Molecular Charge Distributions: Group Theory without Symmetry
P. G. Mezey 462

The Modeling of Chemical Phenomena Using Topological Indices
D. H. Rouvray 470

Theoretical Study of the Addition of Hydrogen Halides to Olefins: A Comparison between $(HCl)_2$ and $(HF)_2$ Additions to Ethylene
C. Clavero, M. Duran, A. Lledós, O. N. Ventura, and J. Bertrán 481

Bond Critical Points in the Electronic Structures of the Main Group Diatomic Hydrides of Lithium through Bromine
R. J. Boyd and K. E. Edgecombe 489

Some Methods and Applications of Electron Density Distribution Analysis
J. P. Ritchie and S. M. Bachrach 499

Quasiperiodization in Classical Hyperchaos
O. E. Rössler and M. Hoffmann 510

Innate Degree of Freedom of a Graph
D. J. Klein and M. Randić 516

Graph Generators
M. Randić, W. L. Woodworth, A. F. Kleiner, and H. Hosoya 522

Stereotopological Indices for a Family of Chemical Graphs
K. C. Millett 536

Computer Enumeration and Generation of Physical Trees
J. V. Knop, W. R. Müller, K. Szymanski, H. W. Kroto, and N. Trinajstić . 549

Towards a Quantum Chemical Software Package Utilizing Transferable Fragments as Molecular Building Blocks
G. Náray-Szabó, G. Kramer, P. Nagy, S. Kugler 555

Volume 8 Number 5 July/August 1987

An Algorithm for Geometry Optimization Without Analytical Gradients
Jon Baker 563

An Objective Computer-Oriented Method for the Calculation of Formation Constants from the Formation Function. A Weighted Least-Squares Curve Fitting
Yousry L. Sidrak and A. Aboul-Seoud 575

The MMP2 Calculational Method
Joseph T. Sprague, Julia C. Tai, Young Yuh, and Norman L. Allinger ... 581

Configurational Specificity of Stacking Interactions in DNA Base Pairs: A Computational Analysis
Nitisch K. Sanyal, M. Roychoudhury, (Kim) Kavita R. Ruhela, and Sugriva Nath Tivari 604

Fast Vector-Scalar-Multiply-and-Add Subroutines for VAX Computers
Gerardo Cisneros, Carlos F. Bunge, and C. C. J. Roothaan 618

Algorithm for Rapid Calculation of Hessian of Conformational Energy Function of Proteins by Supercomputer
Hiroshi Wako and Nobuhiro Go 625

Strategies for Vectorizing the Sparse Matrix Vector Product on CRAY XMP, CRAY 2, and CYBER 205
Charles W. Bauschlicher, Jr. and Harry Partridge 636

A Specific Inhibitor Design Approach by Means of Molecular Dynamics Calculation for Porcine Pancreatic Elastase
T. Fujita 645

Strain Energy Minimization Study of the Mechanism of, and the Barrier to, Conformational Interconversion in Five-Membered Diamine Chelate Rings
Trevor W. Hambley 651

Molecular Valence Calculations of Cyclohexasulfur, Cycloheptasulfur, and Cyclooctasulfur
Risto S. Laitinen, Bruce Randolph, and Tapani A. Pakkanen 658

Basis Sets for Molecular Interactions. 1. Construction and Tests on $(HF)_2$ and $(H_2O)_2$
Zdzislaw Latajka and Steve Scheiner 663

Basis Sets for Molecular Interactions. 2. Application to H_3N—HF, H_3N—HOH, H_2O—HF, $(NH_3)_2$, and H_3CH—OH_2
Zdzislaw Latajka and Steve Scheiner 674

Two Approaches to the Calculation of Molecular Resonance States: Solution of Scattering Equations and Matrix Diagonalization
M. V. Basilevsky and V. M. Ryaboy 683

The Inverse Problem of Isomer Enumeration
Werner Hässelbarth 700

Molecular Graphs as Topological Objects in Space
Jonathon Simon 718

Hartree Fock Instabilities of Sulfur-Nitrogen Systems: S_2N_2
W. G. Laidlaw and M. Benard 727

Ab-Initio MRD-CI Calculations on >A—NO_2 Decomposition Pathway of Nitrobenzene
Joyce J. Kaufman, P. C. Hariharan, Szczepan Roszak, and Marc van Hemert 736

Hamiltonian Dynamics of Chemical Reactions. Consecutive First-Order Reactions and Reactions Possessing One Autocatalytic Intermediate
T. Georgian, J. M. Halpin, and G. L. Findley 744

Volume 8 Number 6 September 1987

Column Design. 3. Theoretical Studies of a Chiral Stationary Phase Used in Column Chromatography
K. B. Lipkowitz, D. A. Demeter, C. A. Parish, and J. M. Landwer 753

Ab initio Study of the He(^{1}S)-Li_2($\tilde{X}$,$^1\Sigma_g^+$) Interaction by the SCF and MP2 Methods
M. A. Matias and A. J. C. Varandas 761

CNDO Force Constants for Glucose
D. M. Back and P. L. Polavarapu 772

Electrostatic Interaction of a Solute with a Continuum. Improved Description of the Cavity and of the Surface Cavity Bound Charge Distribution
J. L. Pascual-Ahuir, E. Silla, J. Tomasi, and R. Bonaccorsi 778

A Study of Basis Set Effects on Structures and Electronic Structures of Phosphine Oxide and Fluorophosphine Oxide
A. Streitweiser, Jr., R. S. McDowell, and R. Glaser 788

Theoretical Studies on the Acid Hydrolysis of Methyl Carbamate
I. Lee, C. K. Kim, and B. C. Lee 794

Molecular Dynamics Simulation of the 1:1 Enzyme-Ligand Complex between Porcine Pancreatic Elastase and Acetyl-Alanine-Proline-Alanine
T. Fujita and E. F. Meyer, Jr. 801

Basis Set and Correlation Effects on Computed Positive Ion Hydrogen Bond Energies of the Complexes $AH_n \cdot AH_{n+1}^{+1}$: AH_n = NH_3, OH_2, and FH
J. E. Del Bene 810

Towards a Valence-Orbital/Bond-Orbital Description of Biochemical H-Bonds from *Ab Initio* Calculations
F. Zuccarello and G. Del Re 816

Revised Algorithms for the Build-Up Procedure for Predicting Protein Conformations by Energy Minimization
K. D. Gibson and H. A. Scheraga 826

Improvement of the Hydrogen Bonding Correction to MNDO for Calculations of Biochemical Interest
A. Goldblum 835

Topology of Conical Intersections and Jahn-Teller Crossing: Application to the Standard Model for XY_4 Molecules in T_2 Ground States
D. Liotard and M. Roche 850

Molecular Orbital Theory of the Properties of Inorganic and Organometallic Compounds. 5. Extended Basis Sets for First-Row Transition Metals
K. D. Dobbs and W. J. Hehre 861

Molecular Orbital Theory of the Properties of Inorganic and Organometallic Compounds. 6. Extended Basis Sets for Second-Row Transition Metals
K. D. Dobbs and W. J. Hehre 880

Atomic Charges Derived from Electrostatic Potentials: A Detailed Study
L. E. Chirlian and M. M. Francl 894

Computer Enumeration of Polyhexes Using the Compact Naming Approach
J. Cioslowski 906

Volume 8 Number 7 October/November 1987

Monte Carlo Study of the Aqueous Hydration of Dimethylphosphate Conformations
B. Jayaram, M. Mezei, and D. L. Beveridge 917

Voronoi Binding Site Models
Gordon M. Crippen 943

On Color Polynomials of Fibonacci Graphs
Sherif El-Basil 956

Fast Matrix Multiplication
Carlos F. Bunge and Gerardo Cisneros 960

A Note on the Efficient and Accurate Computation of the Phase Functions ϕ and χ in Semiclassical Approximations
Peter Senn 965

Determination of an Empirical Energy Function for Protein Conformational Analysis by Energy Embedding
Gordon M. Crippen and P. K. Ponnuswamy 972

Gaussian Basis Sets for the Fifth Row Elements, Mo-Cd, and the Sixth Row Elements W-RN
Odd Gropen 982

Application of SINDO1 to Sulphur Compounds
Karl Jug and Rüdiger Iffert 1004

An Efficient Newton-like Method for Molecular Mechanics Energy Minimization of Large Molecules
Jay W. Ponder and Frederic M. Richards 1016

A Powerful Truncated Newton Method for Potential Energy Minimization
Tamar Schlick and Michael Overton 1025

Application of SINDO1 to Chlorine and Sodium Compounds
Karl Jug and Joachim Schulz 1040

On the Out-of-Plane Deformation of Aromatic Rings, and Its Representation by Molecular Mechanics
Tommy Liljefors, Julia C. Tai, Shusen Li, and Norman L. Allinger 1051

Refined ab initio 6-31G Split-Valence Basis Set Optimization of the Molecular Structures of Biphenyl in Twisted, Planar, and Perpendicular Conformations
Günter Häfelinger and Claus Regelmann 1057

Book Review
Kevin E. Gilbert 1066

Information for Contributors 1068

Volume 8 Number 8 December 1987

Systematic Drug Receptor Mapping: A New Approach to the Analysis of Conformational Energy Calculations of Flexible Molecules with Application to Dopaminergic and Adrenergic Agonists
L. Sanathanan, E. Danaher, K.-H. Kim, and Y. Martin 1075

Molecular Orbital Calculations on Solvents and Other Small Molecules: Correlation between Electronic and Molecular Properties μ, α_{MCL}, π^* and β
D. F. V. Lewis 1084

Cooperative Effects in Extended Hydrogen Bonded Systems Involving O—H Groups. *Ab Initio* Studies of the Cyclic S_4 Water Tetramer
J. E. H. Koehler, W. Saenger, and B. Lesyng 1090

On the Use of Constraints in Molecular Mechanics. II. The Lagrange Multiplier Method and Non-Full-Matrix Newton-Raphson Minimization.
J. L. M. Dillen 1099

Molecular Mechanics Study of Myelin Basic Protein
R. D. Gilliom and G. L. Stoner 1104

An Evaluation of the Performance of Diffuse Function-Augmented Basis Sets for Second Row Elements, Na-Cl
G. W. Spitznagel, T. Clark, P.v.R. Schleyer, and W. J. Hehre 1109

Semi-Empirical Calculations of Molecular Trajectories: Method and Applications to Some Simple Molecular Systems
J. J. P. Stewart, L. P. Davis, and L. W. Burggraf 1117

Nonbonded Interactions. 1. Anisotropic Hydrogen-Hydrogen Interactions
K. B. Wiberg and M. A. Murcko 1124

Calculation of Enthalpies of Hydrogenation of Hydrocarbons
M. R. Ibrahim, Z. A. Fataftah, P.v.R. Schleyer, and P. D. Stout 1131

Benzene-Benzene (Phenyl-Phenyl) Interactions in MM2/MMP2 Molecular Mechanics Calculations
I. Pettersson and T. Liljefors 1139

Benzene, Aromatic Rings, Van der Waals Molecules, and Crystals of Aromatic Molecules in Molecular Mechanics (MM3)
N. L. Allinger and J.-H. Lii 1146

MNDO Calculations on [n] Metacyclophanes
L. W. Jenneskens, F. J. J. de Kanter, W. H. de Wolf, and F. Bickelhaupt 1154

An Investigation of the Relative Stabilities of the Isomers of CF_2N_2: Comparison of *ab initio* and MNDO Calculations
C. Glidewell, D. Higgins, and C. Thomson 1170

Ab Initio Program for Treatment of Related Molecules II. Integral Transformation in Extended Systems
C. Kozmutza 1179

The Hylleraas-CI Method in Molecular Calculations: Two-Electron Integrals
A. Largo-Cabrerizo and E. Clementi 1191

An Analysis of the Structural and Energetic Properties of Deozyribose by Potential Energy Methods
T. Schlick, C. Peskin, S. Broyde, and M. Overton 1199

A Force Field for Allenes and for Nonlinear Acetylenes within the MM2 Approximation
N. L. Allinger and A. Pathiaseril 1225

Announcement 1232

Author Index to Volume 8 1233

Subject Index to Volume 8 1238

Information for Contributors 1241

Volume Title Page i

Volume Contents iii